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Efficient methods to Assimilate Satellite Retrievals Based on Information Content, Part 2: Suboptimal Retrieval Assimilation

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Summary

One of the outstanding problems in data assimilation has been and continues to be how best to utilize satellite data while balancing the tradeoff between accuracy and computational cost. A number of weather prediction centers have recently achieved remarkable success in improving their forecast skill by changing the method by which satellite data are assimilated into the forecast model from the traditional approach of assimilating retrievals to the direct assimilation of radiances in a variational framework. The operational implementation of such a substantial change in methodology involves a great number of technical details, e.g., pertaining to quality control procedures, systematic error correction techniques, and tuning of the statistical parameters in the analysis algorithm. Although there are clear theoretical advantages to the direct radiance assimilation approach, it is not obvious at all to what extent the improvements that have been obtained so far can be attributed to the change in methodology, or to various technical aspects of the implementation. The issue is of interest because retrieval assimilation retains many practical and logistical advantages which may become even more significant in the near future when increasingly high-volume data sources become available.

The central question we address here is: how much improvement can we expect from assimilating radiances rather than retrievals, all other things being equal? We compare the two approaches in a simplified one-dimensional theoretical framework, in which problems related to quality control and systematic error correction are conveniently absent. By assuming a perfect radiative transfer model and perfect knowledge of radiance and background error covariances, we are able to formulate a nonlinear local error analysis for each assimilation method. Direct radiance assimilation is optimal in this idealized context, while the traditional method of assimilating retrievals is suboptimal because it ignores the cross-covariances between background errors and retrieval errors. We show that interactive retrieval assimilation (where the same background used for assimilation is also used in the retrieval step) is

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equivalent to direct assimilation of radiances with suboptimal analysis weights. By examining the weights in different scenarios, e.g., when the dependence of the retrieval on background information varies, we are able to conclude that the effect of neglecting the cross-covariances in retrieval assimilation is potentially most harmful for vertical modes for which the information content of the background roughly balances the information content of the radiance data.

We illustrate and extend these theoretical arguments with several one-dimensional assimilation experiments, where we estimate vertical atmospheric profiles using simulated data from both the High-resolution InfraRed Sounder 2 (HIRS2) and the future Atmospheric InfraRed Sounder (AIRS). The improvement in analysis accuracy obtained by directly assimilating the radiance data, rather than interactively retrieved profiles, is generally small in our experiments. In case of non-interactive retrievals the results depend very much on the quality of the background information used for the retrieval step. In all cases, the impact of the choice of assimilation method is dwarfed by the effect of changing some of the experimental parameters that control the simulated error characteristics of the data and the background. In practice, of course, the uncertainties in many of these parameters are considerable, since radiative transfer models are far from perfect, and radiance and background error covariances are not accurately known. These issues affect all assimilation methods and must be dealt with in details of implementation, which will then ultimately determine the quality of the assimilation products.

1. Introduction

A data assimilation system (DAS) estimates the state of the atmosphere by combining different types of atmospheric observations with a short-term model forecast (often referred to as the first-guess or background field). Assimilated data types include, for example, *in situ* measurements of temperature, moisture, and wind, obtained from radiosonde soundings. Such conventional observations have a high vertical resolution but their geographical coverage is mostly limited to land areas in the northern hemisphere. Satellite observations, on the other hand, provide a more uniform spatial coverage but are hampered by a relatively poor vertical resolution. This stems from the fact that the satellite-borne instruments measure quantities that are functionals of the atmospheric state variables, such as radiances emitted in certain spectral bands, or integrals of atmospheric refractivity, rather than the state variables themselves.

Two basic approaches have been used to incorporate measurements from remote sounding instruments, such as the TIROS vertical operational sounder (TOVS), in data assimilation systems: (1) Assimilate radiances (either clear, cloudy, or cloud-cleared to remove the effects of cloud) directly; (2) Assimilate geophysical products (retrievals) obtained from the observed radiances. Several operational NWP centers have recently moved from the more traditional approach of assimilating retrieved products to radiance assimilation using a variational approach (*e.g.,* Andersson *et al.* 1994, 1998; Derber and Wu 1998). There are strong indications that the implementation of direct radiance assimilation at the National Centers for Environmental Prediction (NCEP) has resulted in a large positive impact on forecast skill, both in the northern and southern hemispheres (Derber and Wu 1998). However, a number of changes were introduced simultaneously to the NCEP DAS, including improvements in quality control and systematic error correction algorithms. It would be extremely interesting to study the performance of various assimilation techniques by means of a controlled set of experiments using a fixed DAS and a single, quality-controlled input data set with a fixed systematic error correction scheme. G. Paul (*private communication*, 1997) has shown that the assimilation of TOVS retrievals can be dramatically improved with rigorous quality control and that the impact of quality-controlled retrievals can be comparable to that obtained with radiance assimilation.

The shift toward radiance assimilation has resulted in part from theoretical work by Eyre *et al.* (1993), who argued that assimilation of retrieved products amounts to a suboptimal use of the data. Retrievals are produced by combining observations with a prior estimate of the state of the atmosphere, possibly obtained from a forecast model, from climatological data, or from a data base of physically feasible vertical profiles. By assimilating the retrievals rather than the radiances into a DAS, additional information from the prior estimate will enter the system along with the measurement information. Errors in retrievals partly depend on the errors in the prior estimate used to produce them, and it is reasonable to expect that the latter are correlated with the errors in the background field used for the assimilation. The resulting cross-covariances between retrieval and background errors are not easily quantified and usually ignored in the assimilation. Clearly, if the retrieval strongly depends on prior information, and if the retrieval errors are misrepresented in the assimilation system, then the assimilation will be suboptimal.

In selecting an appropriate assimilation method, computational and other practical issues must be considered as well. Even if radiance assimilation is more desirable from a theoretical point of view, the computational cost of assimilating retrievals can be significantly less. This is especially pertinent for advanced sounding instruments such as the Atmospheric InfraRed Sounder (AIRS), which will fly on NASA's Earth Observing System PM Platform, and the Infrared Atmospheric Sounding Interferometer (IASI), to fly on the European Meteorological Satellite (EUMETSAT) Polar System. These instruments have one or two orders of magnitude more spectral channels available than TOVS. Because of this dramatic increase in data volume, computational costs and simplified logistics may ultimately be the decisive factors in choosing an appropriate assimilation strategy for these instruments. A dedicated science team has been formed for the AIRS instrument whose task in part is to produce high-quality retrieved products that could be used for data assimilation. Combining the experience, expertise, and algorithm development of data assimilation centers and instrument teams would be highly beneficial to both groups.

In Joiner and da Silva (1998), referred to as Part I in this article, we explored various alternatives to radiance assimilation, with an eye toward the assimilation of future data from advanced sounding instruments. For data assimilation systems such as the Physical-space Statistical Analysis System (PSAS) that has been developed at the NASA Goddard Data Assimilation Office (DAO), the computational cost goes up dramatically as the number of observations increases. Therefore, we focused in Part I on methods to compress the radiance information from high spectral resolution instruments. For AIRS and IASI, the cost of assimilating radiances will be significantly greater than that of assimilating retrievals in a PSAS-type DAS. The number of AIRS and IASI radiance measurements for temperature soundings can be 50 times larger than the number of useful pieces of information for a DAS. We showed in Part I that a compact representation of a retrieved product can be defined from which the retrieval prior information has been largely removed. The information content of the compact retrieval is essentially the same as that of the original set of radiance measurements. Consequently, the assimilation of compact retrievals (or compressed radiances) results in nearly optimal analyses, while retaining some of the practical advantages of traditional retrieval assimilation.

In the present paper we address the following question: how much deterioration actually results from a suboptimal assimilation of retrieved products, due to correlations between retrieval and forecast errors? Starting from the nonlinear statistical analysis equations, we compare the analysis errors obtained by suboptimal assimilation of retrievals (*i.e.*, by neglecting to account for the cross-covariances between retrieval and background errors) with the errors that would result from optimal radiance assimilation. We consider *interactive retrievals*, for which the retrieval prior estimate is identical to the background used in the assimilation, as a special case. The error analysis is illustrated with one-dimensional assimilation experiments using simulated data from high- and low-resolution infrared sounders.

The outline of the paper is as follows. In section 2 we present a general error analysis for various assimilation methods. We first review the statistical analysis equations for nonlinear observation operators. We then apply these equations to the error analysis of radiance assimilation. We briefly discuss the production of 1D retrievals, followed by the error analysis for retrieval assimilation. We then show that in the 1D case, suboptimal assimilation of interactive retrievals is equivalent to direct radiance assimilation with a modified (and therefore suboptimal) gain. This result allows us to assess the impact on analysis errors of cross-covariances between retrieval and background errors. In section 3 we describe the configuration and results of our numerical experiments. We briefly discuss our conclusions and future work in section 4.

2. Error analysis for various assimilation methods

Here we derive approximate expressions for the analysis error covariances associated with the direct assimilation of radiances on the one hand and with the suboptimal assimilation of 1D retrievals on the other. We are primarily concerned with the impact of neglecting the cross-covariances between retrieval and background errors in retrieval assimilation. In practice, of course, there are many additional approximations involved in assimilating remotely sensed data. Minimum-variance assimilation of observations into a DAS requires the complete specification of observation and background error covariances, which are—at best—only approximately known. However in this section we assume that both the observation error covariance (including both instrument and transfer model errors) and the background error covariance are known. This implies the possibility of *optimal* direct radiance assimilation.

The resulting analysis error covariance can then be regarded as a lower bound or benchmark for other assimilation methods.

(*a*) *Nonlinear statistical analysis*

The objective of statistical analysis is to produce a statistically accurate estimate of the atmospheric state, given a set of observations and a background usually in the form of a short-term forecast. The variational framework (*e.g.,* Lorenc 1986; Talagrand 1988) provides an estimate of the state by minimizing the functional

$$J(\mathbf{w}) = (\mathbf{w}-\mathbf{w}^f)^T(\mathbf{P}^f)^{-1}(\mathbf{w}-\mathbf{w}^f) + (\mathbf{w}^o-\mathbf{h}(\mathbf{w}))^T\mathbf{R}^{-1}(\mathbf{w}^o-\mathbf{h}(\mathbf{w})), \tag{1}$$

where the unknown vector $\mathbf{w}$ represents the 3D state of the atmosphere, $\mathbf{w}^f$ is the background estimate (first guess), $\mathbf{w}^o$ is the observation vector, $\mathbf{P}^f$ is the background error covariance matrix, $\mathbf{R}$ is the observation error covariance matrix, and $\mathbf{h}(\mathbf{w})$ is the observation operator (generally nonlinear) that maps the 3D atmospheric state into observables. If the background and observation errors are unbiased, normally distributed, and uncorrelated with each other, and if the covariances $\mathbf{P}^f$ and $\mathbf{R}$ are correctly specified, then the analysis state obtained by minimizing $J(\mathbf{w})$ is the mode of the conditional probability density function $p(\mathbf{w}|\mathbf{w}^f \bigcup \mathbf{w}^o)$ (Jazwinski 1970).

The minimum of $J(\mathbf{w})$ can be obtained by a quasi-Newton iteration of the form

$$\mathbf{w}_{i+1} = \mathbf{w}^f + \mathbf{K}_i\left[\mathbf{w}^o - \mathbf{h}(\mathbf{w}_i) + \mathbf{H}_i(\mathbf{w}_i - \mathbf{w}^f)\right], \tag{2}$$

(*e.g.,* Rodgers, 1976) where the subscript i denotes the iteration, $\mathbf{K}$ is the Kalman gain matrix given by

$$\mathbf{K}_i = \mathbf{P}^f\mathbf{H}_i^T\left(\mathbf{H}_i\mathbf{P}^f\mathbf{H}_i^T + \mathbf{R}\right)^{-1}, \tag{3}$$

and $\mathbf{H}_i$ is a linearized version of h, *i.e.,*

$$\mathbf{H}_i = \left.\frac{\partial \mathbf{h}(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}_i}. \tag{4}$$

The analysis vector, $\mathbf{w}^a$, is the state obtained at convergence:

$$\mathbf{w}^a = \lim_{i\to\infty} \mathbf{w}_i. \tag{5}$$

At convergence, (2) becomes

$$\begin{aligned} \mathbf{w}^a &= \mathbf{w}^f + \mathbf{K}\left[\mathbf{w}^o - \mathbf{h}(\mathbf{w}^a) + \mathbf{H}(\mathbf{w}^a - \mathbf{w}^f)\right] \\ &= \mathbf{w}^f + \mathbf{K}\left[\mathbf{w}^o - \mathbf{H}\mathbf{w}^f\right] - \mathbf{K}\left[\mathbf{h}(\mathbf{w}^a) - \mathbf{H}\mathbf{w}^a\right], \end{aligned} \tag{6}$$

where

$$\mathbf{K} = \mathbf{P}^f\mathbf{H}^T\left(\mathbf{H}\mathbf{P}^f\mathbf{H}^T + \mathbf{R}\right)^{-1}, \tag{7}$$

$$\mathbf{H} = \left.\frac{\partial \mathbf{h}(\mathbf{w})}{\partial \mathbf{w}}\right|_{\mathbf{w}=\mathbf{w}^a}. \tag{8}$$

We will refer to equations (6–8) collectively as the *nonlinear analysis equations.*

If the observation operator is linear, then the matrix $\mathbf{H}$ is constant and $\mathbf{h}(\mathbf{w}) = \mathbf{H}\mathbf{w}$ (only a single iteration of (2) is needed in that case). The analysis equation (6) then becomes

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}\left[\mathbf{w}^o - \mathbf{H}\mathbf{w}^f\right], \tag{9}$$

. If we now consider the possibility of cross-covariance between background and observation errors, denoted by $\mathbf{X}$, it follows that the analysis error covariance $\mathbf{P}^a$ is

$$\begin{aligned} \mathbf{P}^a &= (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^f(\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T \\ &+ \mathbf{K}\mathbf{X}(\mathbf{I} - \mathbf{K}\mathbf{H})^T + (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{X}^T\mathbf{K}^T. \end{aligned} \tag{10}$$

This expression is valid for any gain matrix $\mathbf{K}$ (*e.g.,* for the optimal gain given by (7) or any suboptimal gain). If background and observation errors are uncorrelated, then $\mathbf{X} = 0$ and (10) reduces to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^f(\mathbf{I} - \mathbf{K}\mathbf{H})^T + \mathbf{K}\mathbf{R}\mathbf{K}^T. \tag{11}$$

If, in addition, $\mathbf{K}$ is given by (7), then this expression further reduces to

$$\mathbf{P}^a = (\mathbf{I} - \mathbf{K}\mathbf{H})\mathbf{P}^f. \tag{12}$$

In case of a nonlinear observation operator this error analysis is inexact, due to the presence of the term $\mathbf{K}[\mathbf{h}(\mathbf{w}^a) - \mathbf{H}\mathbf{w}^a]$ in (6). The expressions (10–12) can be used to approximate the actual analysis error covariances when the linearized observation operator $\mathbf{H}$ is evaluated at $\mathbf{w} = \mathbf{w}^a$, as in (8). The local accuracy of the approximations then depends on the magnitude of the linearization error $[\mathbf{h}(\mathbf{w}) - \mathbf{H}\mathbf{w}]$ at $\mathbf{w} = \mathbf{w}^a$.

(*b*) *Optimal direct radiance assimilation*

The observation operator associated with radiance measurements involves an approximate radiative transfer or empirical model, which we denote by $f(\mathbf{z}, \mathbf{b})$. This model can be used to simulate radiances given any state $\mathbf{z}$. The vector $\mathbf{b}$ represents state-independent model parameters. The state variables $\mathbf{z}$ of the radiative transfer model are generally compatible with the state variables $\mathbf{w}$ of the background—in the sense that both vectors are discrete representations of the same geophysical quantities in the same physical domain. However, $\mathbf{z}$ and $\mathbf{w}$ are not necessarily defined at the same locations, so that interpolation is needed to change from one state representation to another. The observation operator associated with radiance assimilation is therefore

$$\mathbf{h}(\mathbf{w}) = \mathbf{f}(\mathbf{z}, \mathbf{b}) = \mathbf{f}(\mathcal{I}\,\mathbf{w}, \mathbf{b}), \tag{13}$$

where $\mathcal{I}$ is an interpolation operator that maps forecast model state variables to the state representation of the radiative transfer model. The linearized observation operator $\mathbf{H}$ is then

$$\mathbf{H} = \frac{\partial \mathbf{h}}{\partial \mathbf{w}} = \frac{\partial \mathbf{f}}{\partial \mathbf{z}}\frac{\partial \mathbf{z}}{\partial \mathbf{w}} = \mathbf{F}\mathcal{I}\,, \tag{14}$$

with $\mathbf{F}$ the Jacobian of the radiative transfer model. The nonlinear analysis equations (6–8) applied to radiance assimilation are therefore

$$\begin{aligned}
\mathbf{w}^a &= \mathbf{w}^f + \mathbf{K}^y\left[\mathbf{y} - \mathbf{F}\mathcal{I}\,\mathbf{w}^f\right] - \mathbf{K}^y\left[\mathbf{f}(\mathcal{I}\,\mathbf{w}^a, \mathbf{b}) - \mathbf{F}\mathcal{I}\,\mathbf{w}^a\right], &(15)\\
\mathbf{K}^y &= \mathbf{P}^f\mathcal{I}^T\mathbf{F}^T\left(\mathbf{F}\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T + \mathbf{R}^y\right)^{-1}, &(16)\\
\mathbf{F} &= \left.\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right|_{\mathbf{z}=\mathcal{I}\,\mathbf{w}^a}, &(17)
\end{aligned}$$

where $\mathbf{y}$ is a vector of radiance measurements, and $\mathbf{R}^y$ is the radiance (or equivalent brightness temperature) error covariance accounting for both instrument error and transfer model error, as discussed in Part 1, by Eyre *et al.* (1993), and by Rodgers (1990). If the assumption holds that radiance and background errors are uncorrelated, then the linear approximation (12) applies. The analysis error covariance for optimal direct radiance assimilation, therefore, is approximately

$$\mathbf{P}^a \approx (\mathbf{I} - \mathbf{K}^y\mathbf{F}\mathcal{I}\,)\mathbf{P}^f = (\mathbf{I} - \mathbf{K}^y\mathbf{F}\mathcal{I}\,)\mathbf{P}^f(\mathbf{I} - \mathbf{K}^y\mathbf{F}\mathcal{I}\,)^T + \mathbf{K}^y\mathbf{R}^y(\mathbf{K}^y)^T. \tag{18}$$

The accuracy of this approximation depends on the size of the transfer model linearization error $[\mathbf{f}(\mathbf{z},\mathbf{b})-\mathbf{f}(\mathbf{z}^a,\mathbf{b})-\mathbf{F}(\mathbf{z}-\mathbf{z}^a)]$ at $\mathbf{z}=\mathcal{I}\,\mathbf{w}^a$. The expression (18) serves as a lower bound for other, suboptimal, assimilation methods.

(c) *Production of optimal 1D retrievals*

A satellite-based remote sounding instrument measures radiances in a number of spectral intervals for each pixel in the instrument field-of-view. For both nadir and limb viewing instruments, these radiances can then be used to estimate (or retrieve) a vertical profile of atmospheric parameters such as temperature or humidity. A prior state estimate is needed to supplement the measurement information if the observing system does not completely resolve the vertical structure of the profile. The physics of radiative transfer generally make nadir viewing instruments insensitive to the high frequency components of the atmosphere's vertical structure. Therefore, retrievals produced from nadir sounding microwave and infrared instruments such as the TOVS may include a significant amount of information from the prior estimate.

The retrieval process is analogous to the general data assimilation problem described in section 2. That is, the retrieval $\mathbf{z}^r$ is a state estimate obtained by combining radiance measurements $\mathbf{y}$ with a prior state estimate (or background) $\mathbf{z}^p$, by means of an estimator $\mathbf{D}$:

$$\mathbf{z}^r=\mathbf{D}\left(\mathbf{y},\mathbf{b},\mathbf{z}^p\right). \tag{19}$$

The retrieval $\mathbf{z}^r$ can be regarded as a one-dimensional analysis of the atmospheric state. In practice (19) is solved repeatedly, using different subsets of the radiance observations, to produce a set of vertical profiles defined at the horizontal locations within the satellite swath.

Errors associated with 1D retrievals defined at different locations are not independent. It can be shown (*e.g.,* Part I) that

$$\mathbf{R}^z\approx\left(\mathbf{I}-\mathbf{D}_y\mathbf{F}\right)\mathbf{P}^p\left(\mathbf{I}-\mathbf{D}_y\mathbf{F}\right)^T+\mathbf{D}_y\mathbf{R}^y\mathbf{D}_y^T, \tag{20}$$

is a linear approximation to the retrieval error covariance, where

$$\mathbf{D}_y=\left.\frac{\partial\mathbf{D}}{\partial\mathbf{y}}\right|_{\mathbf{z}=\mathbf{z}^r}, \tag{21}$$

and $\mathbf{P}^p$ is the error covariance associated with the prior state estimate. The latter involves horizontal as well as vertical correlations, and (20) therefore shows that the errors in retrievals at different locations must be correlated as well. Note the analogy between this expression for the retrieval error covariance $\mathbf{R}^z$ and (11); see also Eyre (1987) and Rodgers (1990).

So far we have not made any assumptions about the nature of the retrieval algorithm, symbolically expressed by the operator $\mathbf{D}$ in (19). Given the prior estimate $\mathbf{z}^p$ and independent data $\mathbf{y}$, the optimal nonlinear one-dimensional retrieval $\mathbf{z}^r$ minimizes the likelihood functional

$$J(\mathbf{z}) = (\mathbf{z} - \mathbf{z}^p)^T(\mathbf{P}^p)^{-1}(\mathbf{z} - \mathbf{z}^p) + (\mathbf{y} - \mathbf{f}(\mathbf{z}, \mathbf{b}))^T(\mathbf{R}^y)^{-1}(\mathbf{y} - \mathbf{f}(\mathbf{z}, \mathbf{b})). \tag{22}$$

The analogy with (1), which is a three-dimensional version of (22), is clear. The nonlinear analysis of the previous sections can be applied here as well, and so it follows that the optimal nonlinear 1D retrieval satisfies

$$\begin{aligned}
\mathbf{z}^r &= \mathbf{z}^p + \mathbf{D}_y\left[\mathbf{y} - \mathbf{F}\mathbf{z}^p\right] - \mathbf{D}_y\left[\mathbf{f}(\mathbf{z}^r, \mathbf{b}) - \mathbf{F}\mathbf{z}^r\right], && (23)\\
\mathbf{D}_y &= \mathbf{P}^p\mathbf{F}^T\left(\mathbf{F}\mathbf{P}^p\mathbf{F}^T + \mathbf{R}^y\right)^{-1}, && (24)\\
\mathbf{F} &= \left.\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right|_{\mathbf{z}=\mathbf{z}^r}. && (25)
\end{aligned}$$

The error covariance of the optimal 1D-retrieval is approximately

$$\mathbf{R}^z \approx (\mathbf{I} - \mathbf{D}_y\mathbf{F})\mathbf{P}^p. \tag{26}$$

The accuracy of this approximation depends on the size of the transfer model linearization error $[\mathbf{f}(\mathbf{z}, \mathbf{b}) - \mathbf{F}\mathbf{z}]$ at $\mathbf{z} = \mathbf{z}^r$.

In practice the retrieval error covariance is not computed by either (20) or (26), but rather modeled and/or estimated directly. Da Silva *et al.* (1996) provide empirical evidence for the presence of both horizontally correlated and uncorrelated retrieval error components, consistent with the two terms in (20). They also show how one can estimate the variances of both components, as well as the decorrelation length of the horizontally correlated component, based on the output of a DAS.

(i) *Interactive retrievals*

Interactive retrievals are produced by taking the same background used by the DAS (*i.e.,* a current short-term forecast) as the prior state estimate in the retrieval process. Then

$$\mathbf{z}^p = \mathcal{I}\,\mathbf{w}^f \tag{27}$$

and consequently

$$\mathbf{P}^p = \mathcal{I}\,\mathbf{P}^f \mathcal{I}^T. \tag{28}$$

Substitution into (23–25) defines the optimal interactive 1D retrieval as

$$\mathbf{z}^r = \mathcal{I}\,\mathbf{w}^f + \mathbf{D}_y\left[\mathbf{y} - \mathbf{F}\mathcal{I}\,\mathbf{w}^f\right] - \mathbf{D}_y\left[\mathbf{f}(\mathbf{z}^r, \mathbf{b}) - \mathbf{F}\mathbf{z}^r\right] \tag{29}$$

$$\mathbf{D}_y = \mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T\left(\mathbf{F}\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T + \mathbf{R}^y\right)^{-1}, \tag{30}$$

$$\mathbf{F} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right|_{\mathbf{z}=\mathbf{z}^r}. \tag{31}$$

Using (26) and (28), the retrieval error covariance $\mathbf{R}^z$ is approximately

$$\mathbf{R}^z \approx (\mathbf{I} - \mathbf{D}_y\mathbf{F})\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T. \tag{32}$$

It follows directly from the linear part of (29) that the retrieval/background error cross-covariance $\mathbf{X}$ is approximately

$$\mathbf{X} \approx (\mathbf{I} - \mathbf{D}_y\mathbf{F})\mathcal{I}\,\mathbf{P}^f. \tag{33}$$

Note that (32, 33) together imply

$$\mathbf{R}^z \approx \mathbf{X}\mathcal{I}^T, \tag{34}$$

which would be exact in case of a linear radiative transfer model $\mathbf{f}$. From (34) it is clear that, in the general, nonlinear case, the retrieval-forecast error cross-covariance can be of the same order of magnitude as the covariance of the retrieval error itself.

(*d*) *Retrieval assimilation*

In traditional retrieval assimilation the retrievals $\mathbf{z}^r$ are simply treated as observations of the atmospheric state $\mathbf{w}$. The observation operator is then linear:

$$\mathbf{h}(\mathbf{w}) = \mathcal{I}\,\mathbf{w}, \tag{35}$$

since it merely involves interpolation from the forecast model state representation to the retrieval state representation. The analysis is then simply

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^z \left[\mathbf{z}^r - \mathcal{I}\,\mathbf{w}^f\right], \tag{36}$$

where $\mathbf{K}^z$ is the gain matrix for retrieval assimilation, which we will now examine more carefully.

Although the error analysis for retrieval assimilation is linear, it is complicated by the fact that the retrieval errors partly depend on the errors in the prior state estimate used in the retrieval process. It is likely, even in the case of non-interactive retrievals, that errors in the prior estimate are correlated with errors in the forecast $\mathbf{w}^f$. This could be caused, for example, by a common dependence of the estimation errors on the current atmospheric state. Therefore one has to assume in general that the retrieval errors are correlated with the forecast errors as well. Given a retrieval-forecast error cross-covariance $\mathbf{X}$, it can be shown that the optimal gain (in the linear minimum-variance sense) is given by

$$\mathbf{K}^{zo} = \left(\mathbf{P}^f\mathcal{I}^T - \mathbf{X}^T\right)\left(\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T + \mathbf{R}^z - \mathcal{I}\,\mathbf{X}^T - \mathbf{X}\mathcal{I}^T\right)^{-1}. \tag{37}$$

In practice, X is usually neglected because it is difficult to estimate; see, however, da Silva *et al.* 1996. Furthermore, numerical solution of the analysis equations using (37) is complicated when the cross-covariance terms are large, because the matrix $\mathbf{K}^{zo}$ then becomes ill-conditioned. Eyre *et al.* (1993) used the approach of Lorenc *et al.* (1986) to control the associated numerical instabilities, by mapping the 1D retrievals into a reduced space and then modifying both the retrievals and their error variances appropriately.

The (suboptimal) gain $\mathbf{K}^{zso}$ obtained by neglecting $\mathbf{X}$ in (37) is

$$\mathbf{K}^{zso} = \mathbf{P}^f\mathcal{I}^T\left(\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T + \mathbf{R}^z\right)^{-1}. \tag{38}$$

Assimilation of retrievals using a gain matrix of this form has been implemented operationally in a number of data assimilation systems (Goldberg *et al.* 1993; Susskind and Pfaendtner 1989).

We now examine the analysis equations for the assimilation of retrievals with an arbitrary gain matrix $\mathbf{K}^z$. Combining (23–25) with the retrieval analysis equation (36) gives

$$\mathbf{w}^a \quad = \quad \mathbf{w}^f + \mathbf{K}^z\left[\mathbf{z}^p + \mathbf{D}_y\left(\mathbf{y} - \mathbf{F}\mathbf{z}^p\right) - \mathcal{I}\,\mathbf{w}^f\right] - \mathbf{K}^z\mathbf{D}_y\left[\mathbf{f}(\mathbf{z}^r, \mathbf{b}) - \mathbf{F}\mathbf{z}^r\right], \tag{39}$$

$$\mathbf{F} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right|_{\mathbf{z}=\mathbf{z}^r}. \tag{40}$$

Lacking an explicit relationship between the prior state estimate $\mathbf{z}^p$ used in the retrieval process and the forecast $\mathbf{w}^f$, equation (39) cannot be further simplified. Based on the linear terms in (39), an approximation for the analysis error covariance is given by

$$\begin{aligned} \mathbf{P}^a \approx\ & (\mathbf{I} - \mathbf{K}^z\mathcal{I})\,\mathbf{P}^f\,(\mathbf{I} - \mathbf{K}^z\mathcal{I})^T \\ & + (\mathbf{K}^z - \mathbf{K}^z\mathbf{D}_y\mathbf{F})\,\mathbf{P}^p\,(\mathbf{K}^z - \mathbf{K}^z\mathbf{D}_y\mathbf{F})^T \\ & + (\mathbf{K}^z\mathbf{D}_y)\,\mathbf{R}^y\,(\mathbf{K}^z\mathbf{D}_y)^T \\ & + (\mathbf{I} - \mathbf{K}^z\mathcal{I})\,\mathbf{P}^{pf}\,(\mathbf{K}^z - \mathbf{K}^z\mathbf{D}_y\mathbf{F})^T \\ & + (\mathbf{K}^z - \mathbf{K}^z\mathbf{D}_y\mathbf{F})\,\mathbf{P}^{pf}\,(\mathbf{I} - \mathbf{K}^z\mathcal{I})^T. \end{aligned} \tag{41}$$

The first three terms in (42) involve error covariances of the forecast, radiance observations, and the prior estimate for the retrieval, respectively. The last two terms involve the cross-covariance $\mathbf{P}^{pf}$ between prior estimation errors and forecast errors.

(i) *Assimilation of interactive retrievals*

Next we specialize to assimilating interactive retrievals, first with an arbitrary gain matrix $\mathbf{K}^z$. Combining (29–31) with the retrieval analysis equation (36) gives

$$\mathbf{w}^a = \mathbf{w}^f + \mathbf{K}^z\mathbf{D}_y\left[\mathbf{y} - \mathbf{F}\mathcal{I}\,\mathbf{w}^f\right] - \mathbf{K}^z\mathbf{D}_y\left[\mathbf{f}(\mathbf{z}^r, \mathbf{b}) - \mathbf{F}\mathbf{z}^r\right], \tag{42}$$

$$\mathbf{D}_y = \mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T\left(\mathbf{F}\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T + \mathbf{R}^y\right)^{-1}, \tag{43}$$

$$\mathbf{F} = \left.\frac{\partial \mathbf{f}}{\partial \mathbf{z}}\right|_{\mathbf{z}=\mathbf{z}^r}. \tag{44}$$

Comparison with the nonlinear analysis equations (15–17) for direct radiance assimilation shows precisely the sense in which the assimilation of interactive retrievals can be regarded as a suboptimal form of direct radiance assimilation.

First, note that the Jacobian $\mathbf{F}$ is evaluated at $\mathbf{z} = \mathcal{I}\,\mathbf{w}^a$ for radiance assimilation but at $\mathbf{z} = \mathbf{z}^r$ for interactive retrieval assimilation. This discrepancy is strictly due to the nonlinearity of the radiative transfer model $\mathbf{f}(\mathbf{z}, \mathbf{b})$. Second, the gain matrix $\mathbf{K}^y$ for radiance assimilation is replaced by $\mathbf{K}^z\mathbf{D}_y$ for retrieval assimilation. This modifies the linear terms of the analysis equation and therefore represents the most significant difference between radiance assimilation and retrieval assimilation.

Let us now assume that the nonlinear component of the radiative transfer model is small, *i.e.,*

$$\mathbf{f}(\delta\mathbf{z}, \mathbf{b}) \approx \mathbf{F}\delta\mathbf{z} \tag{45}$$

for a constant matrix $\mathbf{F}$. This linearity assumption cannot be expected to be uniformly valid (*i.e.,* for all possible retrieval states $\mathbf{z}$), but it should be reasonably accurate locally (*i.e.,* for $\mathbf{z}$ in some neighborhood of $\mathbf{z} = \mathcal{I}\,\mathbf{w}^a$). Using (46) the linearized radiance analysis equations (15–17) are

$$\begin{aligned}
\mathbf{w}^a &= \mathbf{w}^f + \mathbf{K}^y\left[\mathbf{y} - \mathbf{F}\mathcal{I}\,\mathbf{w}^f\right], & (46)\\
\mathbf{K}^y &= \mathbf{P}^f\mathcal{I}^T\mathbf{F}^T\left(\mathbf{F}\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T\mathbf{F}^T + \mathbf{R}^y\right)^{-1}, & (47)
\end{aligned}$$

On the other hand, the linearized interactive retrieval analysis equations (43–45) are

$$\begin{aligned}
\mathbf{w}^a &= \mathbf{w}^f + \mathbf{K}^{y_{so}}\left[\mathbf{y} - \mathbf{F}\mathcal{I}\,\mathbf{w}^f\right], & (48)\\
\mathbf{K}^{y_{so}} &= \mathbf{K}^z\mathcal{I}\,\mathbf{K}^y. & (49)
\end{aligned}$$

The matrix factor $\mathbf{K}^z\mathcal{I}$ multiplying $\mathbf{K}^y$ in (50) reflects the fact that, in general, the assimilation of retrieved products amounts to a suboptimal use of radiance data. A linear approximation for the analysis error covariance associated with interactive retrieval assimilation based on (49) is

$$\mathbf{P}^a \approx (\mathbf{I} - \mathbf{K}^{y_{so}}\mathbf{F}\mathcal{I}\,)\mathbf{P}^f(\mathbf{I} - \mathbf{K}^{y_{so}}\mathbf{F}\mathcal{I}\,)^T + \mathbf{K}^{y_{so}}\mathbf{R}^y(\mathbf{K}^{y_{so}})^T. \tag{50}$$

Note that this expression does not involve the retrieval-forecast error cross-covariance $\mathbf{X}$. To assess the (linear) effect on the analysis error of, for example, neglecting the error cross-covariance terms, (51) can be compared with (18) for optimal direct radiance assimilation.

Consider, for the moment, the optimal retrieval gain $\mathbf{K}^z = \mathbf{K}^{z_o}$ given by (37). Under the linear approximation it follows from (34) that

$$\mathbf{K}^{z_o} = \left(\mathbf{P}^f\mathcal{I}^T - \mathbf{X}^T\right)\left(\mathcal{I}\,\mathbf{P}^f\mathcal{I}^T - \mathcal{I}\,\mathbf{X}^T\right)^{-1}. \tag{51}$$

This expression shows that (47) and (49) would be identical but for the appearance of the interpolation operator $\mathcal{I}$ in several places. This proves the linear equivalence between optimal radiance assimilation and optimal assimilation of optimal 1D retrievals, apart from interpolation effects. As mentioned earlier, however, the optimal retrieval gain is impractical from a computational point of view. Using (34) again we have the alternative expression

$$\mathbf{K}^{z_o} = \left(\mathbf{P}^f \mathcal{I}^T - \mathbf{X}^T\right) \left(\mathcal{I}\, \mathbf{P}^f \mathcal{I}^T - \mathbf{R}^z\right)^{-1}. \tag{52}$$

The second matrix factor on the right-hand side is difficult to invert, unless all its eigenvalues are bounded away from zero. This condition is violated whenever the observing system does not completely resolve the vertical structure of the profile, because in that case there is at least one mode for which the retrieval accuracy is comparable to the forecast accuracy.

Of more practical interest is the following analysis for the suboptimal retrieval gain $\mathbf{K}^z = \mathbf{K}^{z_{so}}$ defined by (38), which was obtained by neglecting the retrieval-forecast error cross-covariances. We consider two extreme cases when (1) the retrievals are completely determined by the radiance observations alone, or (2) the retrievals depend exclusively on the forecast, which is the prior state estimate used in the interactive retrieval process. Substituting (32) into (38), we obtain

$$\mathbf{K}^{z_{so}}\mathcal{I} = \mathbf{P}^f \mathcal{I}^T \left(\mathcal{I}\, \mathbf{P}^f \mathcal{I}^T + (\mathbf{I} - \mathbf{D}_y \mathbf{F})\mathcal{I}\, \mathbf{P}^f \mathcal{I}^T\right)^{-1} \mathcal{I}. \tag{53}$$

Note that $\mathbf{K}^{z_{so}}\mathcal{I}$ is the matrix factor that modifies the optimal gain for the radiance data; see (50). The linear part of the interactive retrieval equation (29) can be written

$$\mathbf{z}^r = [\mathbf{I} - \mathbf{D}_y \mathbf{F}]\, \mathcal{I}\, \mathbf{w}^f + \mathbf{D}_y \mathbf{y}. \tag{54}$$

If the state is overwhelmingly determined by the radiance observations, then $\mathbf{D}_y \mathbf{F} \approx \mathbf{I}$, *i.e.*, the retrieval is almost independent of the prior estimate $\mathbf{w}^f$ (see Part I). Equation (54) then shows that the difference between radiance assimilation and retrieval assimilation is due only to the appearance of the interpolation operator $\mathcal{I}$; neglecting interpolations we have $\mathbf{K}^{z_{so}}\mathcal{I} \approx \mathbf{I}$. This shows, not unexpectedly, that in this case the effect of ignoring the cross-covariance terms in the retrieval assimilation is negligible.

In the other extreme, suppose that the radiance observations contain virtually no information. Then $\mathbf{D}_y \mathbf{F} \approx 0$, and (54) then implies that, ignoring interpolation effects, the radiance data are assigned only half as much weight as they should be. On the other hand, (48) implies that the optimal weights for the radiance data are very small to begin with in this situation, because the radiance errors are so large. Therefore the difference between optimal radiance assimilation and suboptimal retrieval assimilation is negligible in this case as well.

The preceding argument applies to each individual mode of the retrieved state. This implies that the impact of ignoring the cross-covariance terms in interactive retrieval assimilation should be largest for modes that are determined partly by the observations and partly by the forecast information.

3. One-dimensional simulation results

We compare the analysis errors for one-dimensional optimal radiance assimilation with those for several suboptimal retrieval assimilations, using simulated Jacobians for two different infrared sounders: the Atmospheric InfraRed Sounder (AIRS) and the High-resolution InfraRed Sounder 2 (HIRS2). HIRS2 has flown continuously on polar-orbiting satellites from 1978 to the present as part of the TIROS Operational Vertical Sounder or TOVS (see Smith *et al.* 1979). HIRS2 has 19 infrared channels, a single spot ground resolution at nadir of 17.4 km and scans cross-track $\pm 49.5°$ from nadir. AIRS is an advanced sounder with over 2000 channels that will fly on the NASA EOS PM platform in the year 2000 (Aumann and Pagano, 1994). AIRS has similar spatial resolution and coverage as HIRS2, but the spectral resolution is more than an order of magnitude greater.

We focus here on a single aspect of data assimilation for infrared sounders, namely the temperature profile information contained in the radiances. The simulated HIRS2 channel set includes 11 of the 20 channels (channels 1-7 and 13-16). These are affected mainly by CO_2 absorption and are typically used for temperature soundings. The AIRS channel set includes all 550 available channels between 650 and 742 cm^{-1}, between 2160 and 2270 cm^{-1}, and between 2379 and 2407 cm^{-1}. These are the same channel sets used in Part I and we also prescribe the same instrument specified equivalent noise temperatures as in Part I. Some of the HIRS2 and AIRS channels are affected by water vapor absorption and/or the surface skin temperature and emissivity, but for simplicity we assume these variables to be known.

As in Part I, the Jacobian $\mathbf{F}$ for each instrument is computed using a fast radiative transfer algorithm based on parameterizations similar to the ones described in Susskind *et al.* (1983). The linearized observation operator $\mathbf{H}$ is equal to $\mathbf{F}$, because for these one-dimensional experiments $\mathcal{I} = \mathbf{I}$. Radiance errors for different channels are assumed independent, with variances equal to the sum of the squared channel equivalent noise temperatures ($NE\Delta T$) plus an additional $(0.1\mathrm{K})^2$ to account for linearization error. For simplicity, the radiative transfer model is taken to be perfect, and we assume clear-sky night-time (*i.e.*, no reflected solar radiation) and nadir-viewing conditions. These simulations are sufficiently realistic to provide a meaningful comparison between the different assimilation approaches; in particular, the same simplifying assumptions are made in all cases.

We specify a thickness forecast error covariance P^f for our experiments at 18 pressure levels (0.4, 1, 2, 5, 10, 30, 50, 70, 100, 150, 200, 250, 300, 400, 500, 700, 850, and 1000 hPa) based on the Goddard Earth Observing System Data Assimilation System (GEOS DAS) 6-hour forecast height error covariances. These were estimated from time series of North-American rawinsonde observed-minus-forecast residuals using the method described in Dee *et al.* (1998a,b). Horizontal forecast error correlations do not play a role in these experiments. Retrieval error covariances originally specified for temperature have been hydrostatically converted to thickness error covariances.

For radiance assimilation experiments we use the linearized analysis equations (47, 48), and estimate the analysis errors using (18). For interactive retrieval assimilation we use (36, 38), specify retrieval error covariances according to (32, 30), and estimate the analysis errors using (51). In Part I we showed by means of Monte Carlo simulations that the linearized expressions for the analysis error covariances approximate the errors for this particular problem quite well, although the actual errors are slightly underestimated.

(*a*) *Interactive retrieval assimilation*

(i) *Using correct retrieval error covariances*

Figure 1 shows the estimated thickness error standard deviations (in m), as a function of pressure level, for radiance assimilation (solid curves) and for interactive-retrieval assimilation (dashed curves), using either AIRS or HIRS. For reference, the prescribed forecast error standard deviations are shown in the figure as well (dashed-dotted curve). Since the error covariances are correctly specified for this experiment, interactive-retrieval assimilation is suboptimal only because the cross-covariances between retrieval errors and forecast errors are not accounted for. The error standard deviations are obtained from the diagonal of the analysis error covariance $\mathbf{P}^a$ computed for each case. The figure shows that the analysis error standard deviations for the two assimilation methods are virtually indistinguishable. Not shown are the thickness analysis error vertical correlations, which are also nearly identical for the two methods. To gain some insight into this result, we examine separately the contributions to the analysis error covariances of the forecast errors and of the radiance errors.

We project the two components of the analysis error covariance onto the eigenvectors of $\mathbf{F}^T(\mathbf{R}^y)^{-1}\mathbf{F}$, which are the columns of the unitary matrix $\mathbf{U}$ in

$$\mathbf{F}^T(\mathbf{R}^y)^{-1}\mathbf{F} = \mathbf{U}\mathbf{D}\mathbf{U}^T, \tag{55}$$

with $\mathbf{D}$ a diagonal matrix of eigenvalues. This transformation was used in Part I to produce compact Partial Eigen-Decomposition (PED) retrievals. The eigenvectors for the two instruments are shown in Figure 2 in order of decreasing eigenvalue, that is to say, in order of increasing uncertainty. Accordingly we can define

$$\mathbf{A} = \mathbf{U}^T(\mathbf{I} - \mathbf{K}\mathbf{F})\mathbf{P}^f(\mathbf{I} - \mathbf{K}\mathbf{F})^T\mathbf{U} \tag{56}$$

and

$$\mathbf{B} = \mathbf{U}^T\mathbf{K}\mathbf{R}^y\mathbf{K}\mathbf{U}, \tag{57}$$

corresponding to the two terms in (18) and (51). The matrix $\mathbf{A}$ represents the forecast error contribution, and $\mathbf{B}$ the radiance error contribution, to the analysis error covariance. Figure 3 shows the diagonal elements of these two matrices on a logarithmic scale, for the optimal (radiance assimilation) case with $\mathbf{K} = \mathbf{K}^y$ given by (48) and the suboptimal (interactive-retrieval assimilation) case with $\mathbf{K} = \mathbf{K}^{y_{so}}$ given by (50) and (38).

Figure 3 shows that the interactive-retrieval assimilation effectively assigns too much weight to the forecast and too little to the radiance data. The leading 7 modes are well determined by the radiance data, so that the analysis errors for these modes are dominated by the radiance errors. The slightly increased weight given to the forecast therefore does not greatly affect the analysis in the leading modes. For the trailing 7 modes the situation is reversed: information from the forecast is dominant, and decreasing the weight given to the radiance data likewise does not significantly affect the analysis. For modes in between these two extremes (modes 8 and 9), the influence of the information in the forecast is comparable to that in the radiances. The change in relative weights in these modes is therefore responsible for most of the analysis degradation in interactive-retrieval assimilation. As shown in Figure 1, however, the overall degradation as measured by analysis error standard deviations in physical space is insignificant.

Figure 4 is similar to Figure 3, but uses the Jacobian and error covariances for the HIRS instrument. The difference in weights in the cross-over modes (modes 2-4) appears to be more severe for HIRS than for AIRS. However, as shown in Figure 1, the overall degradation in the suboptimal analysis is small in this case as well.

Table 1 shows the condition numbers of the innovation covariance matrices (*i.e.,* the quantity to be inverted when solving the analysis equation) for radiance assimilation and for optimal and suboptimal retrieval assimilation for AIRS and HIRS. The numerical conditioning of the analysis equations is slightly better for suboptimal retrieval assimilation than for radiance assimilation. This implies that solving the analysis equations (in the PSAS context) will be somewhat more efficient for suboptimal retrieval assimilation than for radiance assimilation. The condition numbers for the innovation covariance associated with the optimal retrieval assimilation gain matrix (37) are very high implying near singularity. This result is expected as explained in section 2 and by Eyre *et al.* (1993) and suggests that it will not be possible to assimilate retrievals from nadir-viewing instruments such as AIRS and HIRS with an optimal gain matrix.

(ii) *Using incorrect retrieval error covariances*

We now examine the effect of specifying incorrect retrieval error covariances in the assimilation. This would occur in practice, for example, if the DAS employs a homogeneous retrieval error covariance model, even though actual retrieval errors are state-dependent. Equations (32, 30) show how the interactive retrieval error covariances depend on the forecast and brightness temperature error covariances, as well as on the Jacobian of the radiative transfer model. The latter is state-dependent due to the nonlinearity of the Planck function, while the brightness temperature errors depend on scene brightness temperature. A colder scene brightness temperature corresponds to a higher equivalent noise temperature. For example, the HIRS2 equivalent noise temperatures for tropical and mid-latitude profiles differ by factors ranging from about 0.8 to 1.6 depending on the channel.

For these experiments we specify the interactive retrieval error covariances using (32, 30) as before, but with Jacobians and brightness temperature error covariances computed for three different model-generated profiles, corresponding to a low, middle, and high-latitude case. These profiles are described in more detail in Part I. We then assimilate, for example, interactive retrievals in the tropics using the retrieval error covariances computed for the mid-latitude profile. The analysis is then suboptimal, not only because cross-covariances between retrieval errors and forecast errors are ignored, but also because the retrieval error covariances are misspecified. We can still estimate the analysis error standard deviations for these cases, by means of (51) with the gain matrix defined by (50,38).

Figure 5 shows the estimated thickness error standard deviations for the tropical assimilation with AIRS and HIRS, with incorrect error covariances based on the mid-latitude profile. Solid curves correspond to (optimal) radiance assimilation, and dashed curves to the (suboptimal) retrieval assimilation. The dotted-dashed curve indicates the forecast error standard deviations. The differences between the analysis errors for the optimal and suboptimal assimilations are insignificant. We obtain similarly small differences for all other profile combinations. These results indicate that, for these one-dimensional simulations, the analyses are not sensitive to small misspecifications of the retrieval error covariance. In the previous section we showed that, in certain regimes, a misspecification of the errors (*e.g.*, neglecting retrieval/background cross-covariance) does not significantly harm the analysis. The results of this section imply that, in addition, a relatively small misspecification of the retrieval error covariance also does not significantly degrade the suboptimal retrieval assimilation. This result supports the use of homogeneous retrieval error covariances for interactive clear-sky temperature retrieval assimilation.

(*b*) *Non-interactive retrieval assimilation*

In order to simulate analysis errors that would obtain with non-interactive retrieval assimilation, we need to make assumptions about the accuracy of the prior state estimate used for the retrieval, and about the cross-covariances between prior estimation errors and the forecast errors; see (42). We are interested in the situation where a forecast model from an older or different DAS or from some other source such as climatology is used as the prior information for the retrieval. For this experiment we take the prior estimation error covariances to be the same as the forecast error covariances, except that the error variances are multiplied by a factor α^2. To model the forecast-prior error covariances, we multiply the covariances that would result if the errors were perfectly correlated by a factor γ. Thus, $\alpha = 1, \gamma = 1$ corresponds to interactive retrieval assimilation. As $\gamma \to 0$ the analysis errors may become smaller than those obtained with direct radiance assimilation, because the prior state estimate then provides another independent source of information for the assimilation. In reality, prior estimation errors and forecast errors are likely to be highly correlated. As $\gamma \to 1$ when $\alpha > 1$, the analysis should degrade as the prior state estimate, which then contains no additional information over the forecast, is assigned too much weight.

The dashed curves in Figure 6 are the estimated analysis errors for the case $\alpha = 1.5, \gamma = 0.75$. As before, solid curves correspond to (optimal) radiance assimilation, and the dotted-dashed curve indicates the forecast error standard deviations. At some altitudes, the HIRS analysis errors actually do exceed the forecast errors. Where the information content of the radiances is high, such as in the lower troposphere, the degradation with respect to the optimal analysis is small.

Figures 7 and 8 show the same curves but now with $\gamma = 0.50$ and $\gamma = 0.25$, respectively. This corresponds to an increase in the amount of independent information contained in the prior state estimate for the retrieval. As expected, the results improve as γ decreases; in fact, when $\gamma = 0.25$ the analysis errors are smaller than those obtained with radiance assimilation at almost every altitude. Finally, Figure 9 shows the results for $\alpha = 2.0, \gamma = 0.75$, corresponding to the use of a relatively inaccurate prior state estimate that is highly correlated with the forecast. Clearly the results are much worse in this case.

4. Conclusions and Future Work

We set out in this paper to compare different ways of utilizing satellite data, either by directly assimilating radiances in a variational framework, or by first producing one-dimensional retrievals and then assimilating the retrievals. Actual implementation of either method in an operational data assimilation system involves numerous technical details, pertaining to quality control, systematic error correction, and covariance tuning. This begs the question whether the recent improvements in forecast skill obtained by centers that implemented direct radiance assimilation, is due to the change in methodology, or a result of various implementation details. In any case, computational and logistical arguments favor some form of retrieval assimilation for future high-volume data types especially for PSAS-like assimilation systems. It is therefore important to learn as much as possible about the expected analysis errors for various suboptimal assimilation schemes, and to investigate whether any negative effects of retrieval assimilation are actually significant in view of the many uncertainties inherent in any data assimilation method.

We presented a theoretical error analysis of the various assimilation methods: direct radiance assimilation, interactive retrieval assimilation, and non-interactive retrieval assimilation. As has been pointed out elsewhere, interactive retrieval assimilation amounts to a suboptimal use of radiance data because cross-covariances between the retrieval and background errors are not accounted for in the assimilation. We showed that, in fact, interactive retrieval assimilation is linearly equivalent to radiance assimilation with modified (hence suboptimal) analysis weights. We then showed that the resulting degradation of analysis accuracy is small for vertical modes that are determined either by the radiances or by the model forecast alone, but that the degradation can be significant for modes that are not well determined by either.

These results were further clarified with a number of one-dimensional numerical experiments, for which we simulated radiance data from two different infrared sounders: the Atmospheric InfraRed Sounder (AIRS) and the High-resolution InfraRed Sounder 2 (HIRS2). We found that the degradation of analysis errors due to the assimilation of interactive retrievals, rather than radiances, is insignificant in the context of these experiments. Moreover, when we misspecified retrieval error covariances in the retrieval assimilation, the degradation was still small. We also reported results from several experiments with the assimilation of non-interactive retrievals, using different assumptions about the accuracy of the prior state estimate used in the retrieval process, and about the cross-covariances between the prior estimation and forecast errors. We found that successful assimilation of non-interactive retrievals requires that the accuracy of the prior state estimates used for the retrievals must be at least comparable to that of the forecast. If not, then the analysis may turn out significantly worse than in the case of either direct radiance or interactive retrieval assimilation. For an instrument that provides only a small impact at best, as is the case for TOVS in the Northern hemisphere, assimilation of retrievals based on inferior prior state estimates may actually produce analyses that are less accurate than the forecast itself.

Our conclusions are based on theoretical considerations combined with simple one-dimensional simulations. We would like to show in future simulations that similar conclusions hold in three dimensions, when horizontal correlations of forecast errors play a role as well. We also plan to include multiple data types in our simulations and finally to compare different assimilation strategies with real data in a full data assimilation system.

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TABLE 1. Condition numbers for the innovation covariance matrix

	AIRS	HIRS
Radiance assimilation	3.25×10^3	7.17×10^2
Retrieval assimilation, neglect **X** (sub-optimal)	5.63×10^2	6.39×10^2
Retrieval assimilation, account for **X** (optimal)	7.59×10^5	7.11×10^8

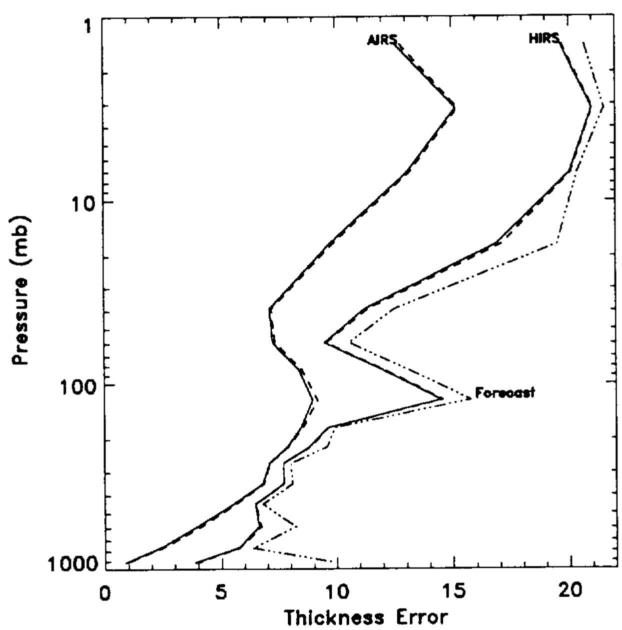

Figure 1. Thickness analysis error standard deviations (in m) for optimal radiance assimilation (solid lines) and for interactive retrieval assimilation (dashed lines), using simulated AIRS and HIRS data. Forecast error standard deviations are shown for reference (dot-dashed line).

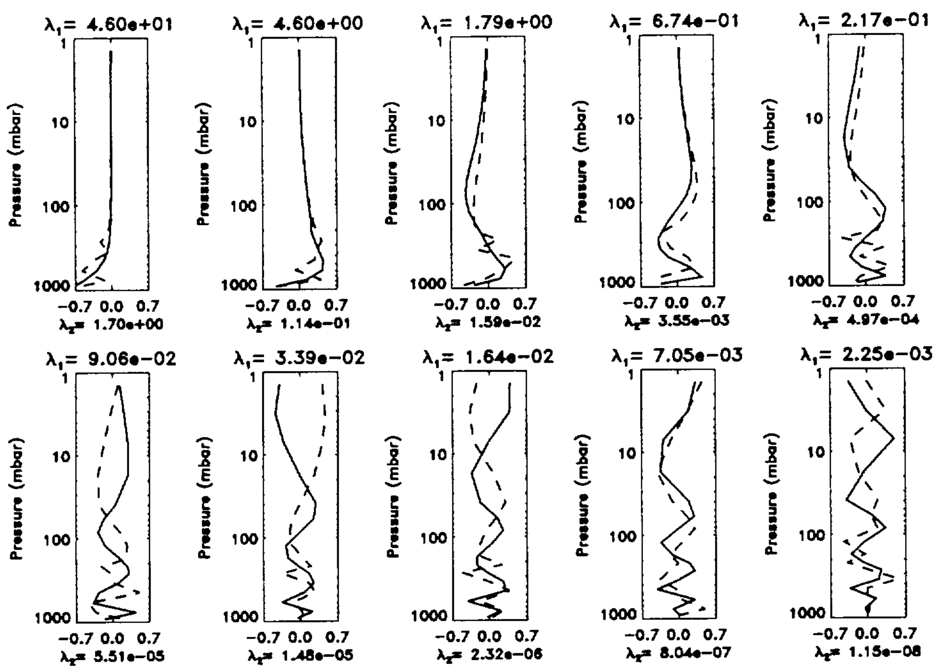

Figure 2. Leading eigenvectors and eigenvalues of $F^T(R^y)^{-1}F$ for AIRS (solid line, λ_1) and HIRS (dashed line, λ_2) for a mid-latitude profile.

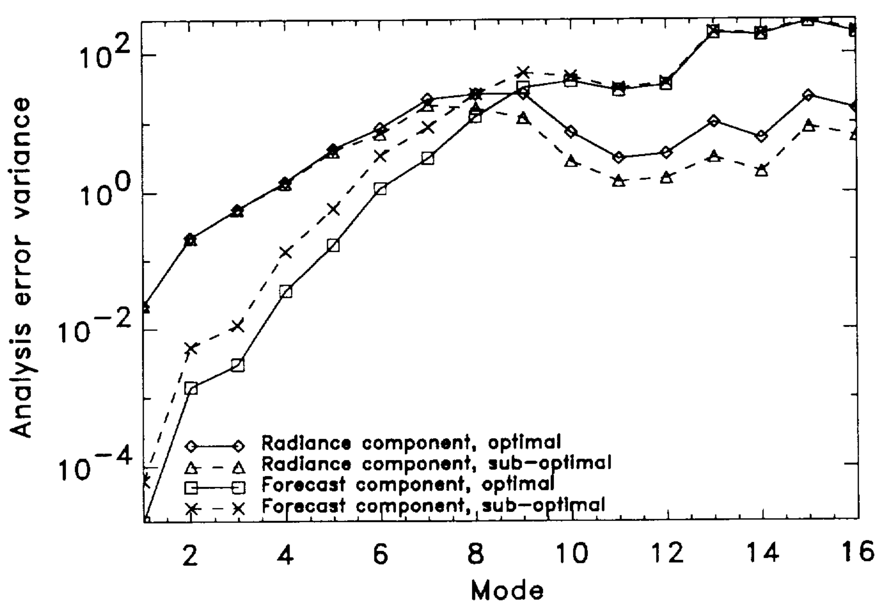

Figure 3. Forecast and radiance contributions to the analysis error variances, projected onto the eigenvectors of Figure 2, for simulated AIRS data.

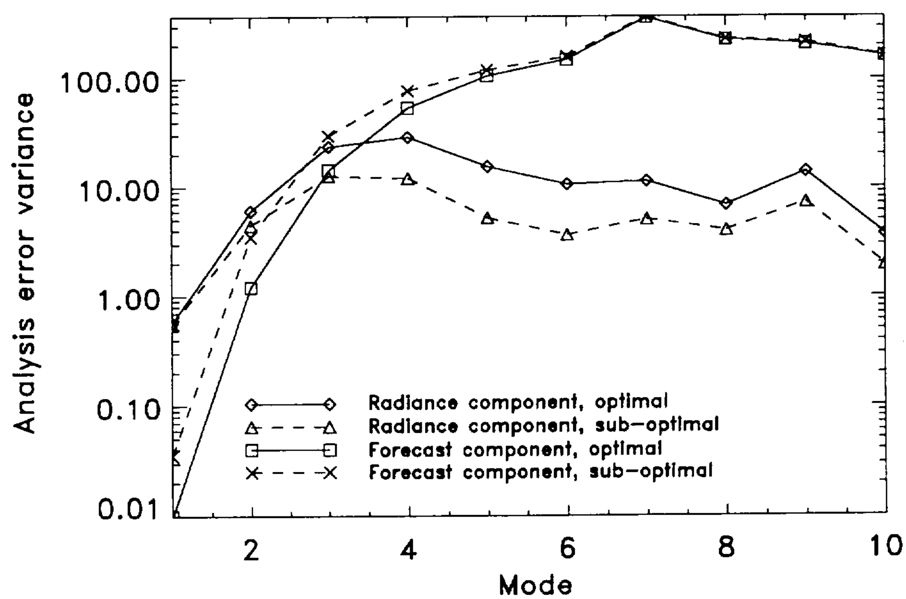

Figure 4. As Figure 3, for simulated HIRS2 data.

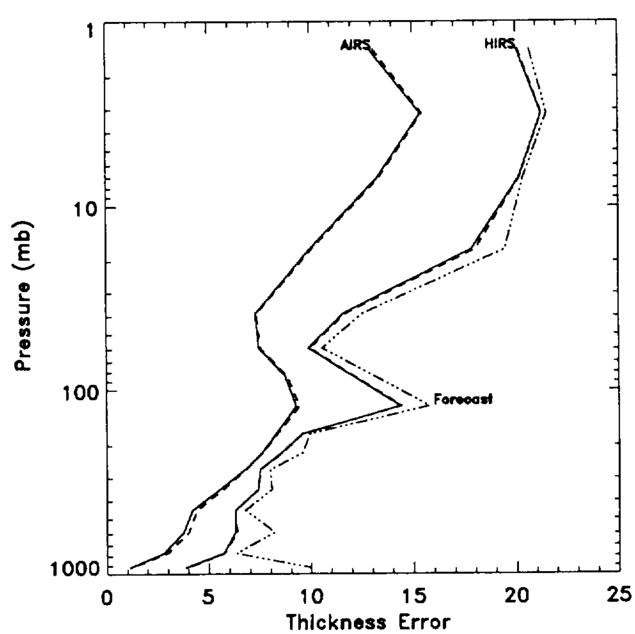

Figure 5. As Figure 1, for a simulated tropical profile. Error covariances for the retrieval assimilation were incorrectly specified as for a mid-latitude profile.

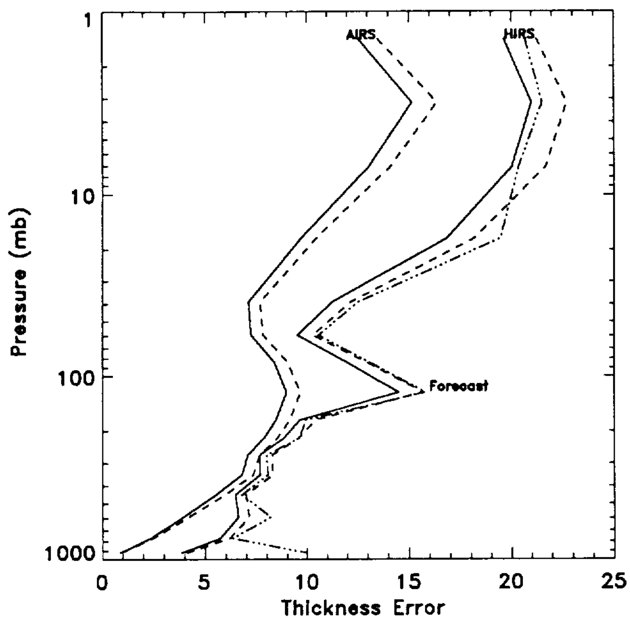

Figure 6. As Figure 1, but for non-interactive retrieval assimilation, using $\alpha = 1.5$, $\gamma = 0.75$ for defining the error covariances.

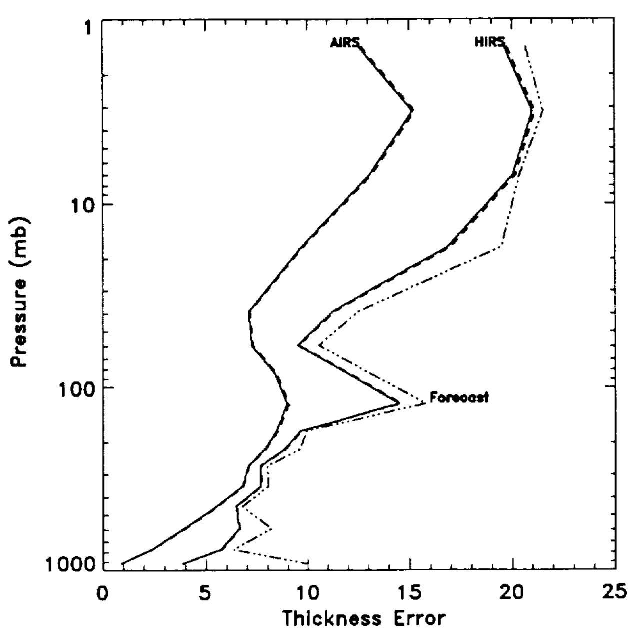

Figure 7. As Figure 1, but for non-interactive retrieval assimilation, using $\alpha = 1.5$, $\gamma = 0.50$ for defining the error covariances.

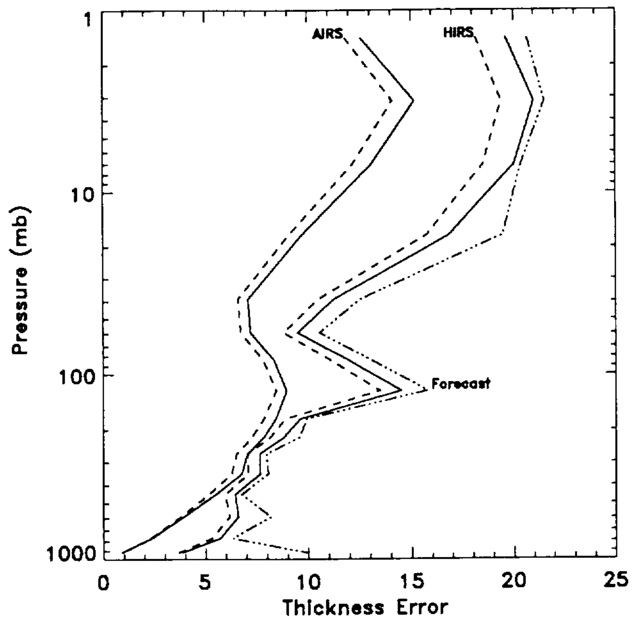

Figure 8. As Figure 1, but for non-interactive retrieval assimilation, using $\alpha = 1.5, \gamma = 0.25$ for defining the error covariances.

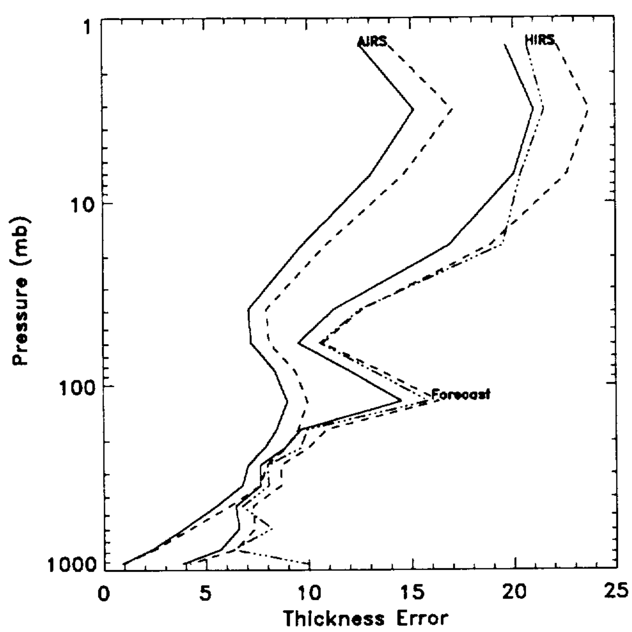

Figure 9. As Figure 1, but for non-interactive retrieval assimilation, using $\alpha = 2.0, \gamma = 0.75$ for defining the error covariances.